REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
11 April 2003	Abstract	

4. TITLE AND SUBTITLE

Polynitrogen Chemistry

5a. CONTRACT NUMBER
F04611-99-C-0025

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Karl Christie, et al.

5d. PROJECT NUMBER
DARP

5e. TASK NUMBER
A205

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

ERC, Inc.
10 E. Saturn Blvd.
Edwards AFB, CA 93524-7680

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRS
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S NUMBER(S)
AFRL-PR-ED-AB-2003-096

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
					Sheila Benner
a. REPORT	b. ABSTRACT	c. THIS PAGE	A		19b. TELEPHONE NUMBER *(include area code)*
Unclassified	Unclassified	Unclassified			(661) 275-5963

FILE

MEMORANDUM FOR PRS (In-House Contractor Publication)

FROM: PROI (STINFO) 21 Apr 2003

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2003-096**
Christe, Karl (ERC) et al., "Polynitrogen Chemistry"

5194

Molecular Dynamics Conference **(Statement A)**
(San Diego, CA, 18-20 May 2003) (Deadline: 08 Apr 2003)

Polynitrogen Chemistry

Karl Christe, William Wilson, Ashwani Vij, Vandana Vij, Robert Corley, Jerry Boatz, Stefan Schneider, Thorsten Schroer, Ross Wagner, Ralf Haiges, David Dixon, David Feller, Mark Gordon, Heather Netzloff, and Don Jenkins

ERC and Space and Missile Propulsion Division, Air Force Research Laboratory Edwards Air Force Base, CA 93524, Loker Research Institute, University of Southern California, Los Angeles, CA 90089, Pacific Northwest National Laboratory, Richland WA 99352, Department of Chemistry, Iowa State University, Ames, IA 50011, and Department of Chemistry, University of Warwick, Coventry CV4 7AL, UK

karl.christe@edwards.af.mil

Under combined DARPA, AFOSR, NSF, and DOE sponsorship, we have continued our work in polynitrogen chemistry. We have successfully prepared and characterized numerous polyazido compounds, such as $As(N_3)_3$, $Sb(N_3)_3$, $As(N_3)_5$, $Sb(N_3)_5$, $As(N_3)_6^-$, $Sb(N_3)_6^-$, $Te(N_3)_4$, $Te(N_3)_6^{2-}$, $P(N_3)_6^-$, and $B(N_3)_4^-$, and have studied the combination of N_5^+ with some of these anions. Most of these compounds are extremely energetic and shock sensitive.

We have studied the reactions of the NF_4^+ and $N_2F_3^+$ cations with HN_3 in HF solution. The synthesis of the N_7^- anion was also pursued by preparing and characterizing R_3SiNCl_2 and $(R_3Si)_2NCl$ compounds. Although their chlorine atoms could not be replaced by azido groups, the reaction of the latter with HF/MF_5 resulted in the isolation of salts of the novel monochloroammonium cation.

Enthalpies of formation were calculated for gas phase N_3, N_3^-, N_5^+, and N_5^- from *ab initio* molecular orbital theory. Stability calculations were carried out for solid $N_5^+N_3^-$ and $N_5^+N_5^-$, using these values and lattice energy estimates.

The possible existence of FN_5 was studied both experimentally by FT-IR spectroscopy of the volatile decomposition products from the thermolysis of $(N_5^+)_2SnF_6^{2-}$ and computationally using a RRKM analysis.